Welcome to STN International Web Page URLs for STN Seminar Schedule - N. America NEWS Apr 08 "Ask CAS" for self-help around the clock NEWS BEILSTEIN: Reload and Implementation of a New Subject Area NEWS 3 Apr 09 NEWS 4 Apr 09 ZDB will be removed from STN NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER Apr 22 Federal Research in Progress (FEDRIP) now available NEWS NEWS 9 Jun 03 New e-mail delivery for search results now available NEWS 10 Jun 10 MEDLINE Reload NEWS 11 Jun 10 PCTFULL has been reloaded NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment USAN to be reloaded July 28, 2002; NEWS 13 Jul 22 saved answer sets no longer valid NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY NEWS 15 Jul 30 NETFIRST to be removed from STN NEWS 16 Aug 08 CANCERLIT reload NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN NEWS 18 Aug 08 NTIS has been reloaded and enhanced NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced NEWS 23 Sep 03 JAPIO has been reloaded and enhanced NEWS 24 Sep 16 Experimental properties added to the REGISTRY file NEWS 25 Sep 16 CA Section Thesaurus available in CAPLUS and CA NEWS 26 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985 NEWS 27 Oct 21 EVENTLINE has been reloaded NEWS 28 Oct 24 BEILSTEIN adds new search fields NEWS 29 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN NEWS 30 Oct 25 MEDLINE SDI run of October 8, 2002 NEWS 31 Nov 18 DKILIT has been renamed APOLLIT NEWS 32 Nov 25 More calculated properties added to REGISTRY NEWS 33 Dec 02 TIBKAT will be removed from STN NEWS 34 Dec 04 CSA files on STN <u>NEWS 35</u> Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date NEWS 36 Dec 17 TOXCENTER enhanced with additional content NEWS 37 Dec 17 Adis Clinical Trials Insight now available on STN NEWS 38 Dec 30 ISMEC no longer available NEWS 39 Jan 13 Indexing added to some pre-1967 records in CA/CAPLUS Jan 21 NUTRACEUT offering one free connect hour in February 2003 NEWS 40 NEWS 41 Jan 21 PHARMAML offering one free connect hour in February 2003 NEWS 42 Jan 29 Simultaneous left and right truncation added to COMPENDEX, ENERGY, INSPEC NEWS 43 Feb 13 CANCERLIT is no longer being updated NEWS 44 Feb 24 METADEX enhancements NEWS 45 Feb 24 PCTGEN now available on STN NEWS 46 Feb 24 TEMA now available on STN NEWS 47 Feb 26 NTIS now allows simultaneous left and right truncation NEWS 48 Feb 26 PCTFULL now contains images NEWS 49 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results NEWS EXPRESS January 6 CURRENT WINDOWS VERSION IS V6.01a, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002 NEWS HOURS STN Operating Hours Plus Help Desk Availability

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FILE 'HOME' ENTERED AT 18:22:05 ON 06 MAR 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION 0.21

FULL ESTIMATED COST

0.21 R 2003

FILE 'REGISTRY' ENTERED AT 18:22:13 ON 06 MAR 2003
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STRUCTURE FILE UPDATES: 5 MAR 2003 HIGHEST RN 497055-63-7 DICTIONARY FILE UPDATES: 5 MAR 2003 HIGHEST RN 497055-63-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP_CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> L1

STRUCTURE UPLOADED

=> d 11

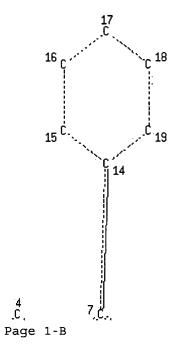
L1 HAS NO ANSWERS

L1

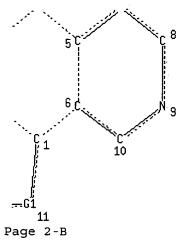
STR

0 20 S 21

Page 1-A



2 C. 13 C. 12 Page 2-A



Page 2-B VAR G1=20/21 NODE ATTRIBUTES: NSPEC IS R

NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AТ	4

```
NSPEC IS R
             AΤ
                    5
NSPEC IS R
              AT
NSPEC IS R
              \mathtt{AT}
                    7
             AT 8
AT 9
AT 10
AT 11
NSPEC IS R
              AT 12
NSPEC IS R
              AT 13
NSPEC IS R AT 14
NSPEC IS R
              AT 15
NSPEC IS R
              AT 16
NSPEC IS R
              AT 17
NSPEC IS R
              AT 18
NSPEC IS R
              AT 19
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
```

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 18:24:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 146 TO 694

PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s 11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 18:24:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 355 TO ITERATE

100.0% PROCESSED 355 ITERATIONS 6 ANSWERS

SEARCH TIME: 00.00.01

L3 6 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 148.95 149.16

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FILE COVERS 1907 - 6 Mar 2003 VOL 138 ISS 10 FILE LAST UPDATED: 5 Mar 2003 (20030305/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 18:22:05 ON 06 MAR 2003)

FILE 'REGISTRY' ENTERED AT 18:22:13 ON 06 MAR 2003

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 6 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 18:24:15 ON 06 MAR 2003

=> s 13

L4 1 L3

=> d 14, ibib abs fhitstr, 1

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS

Full Citing Text References

ACCESSION NUMBER: 2002:51467 HCAPLUS

DOCUMENT NUMBER: 136:118393

TITLE: Preparation and use of furan-fused-4-phenyl

substituted tetrahydroisoquinolines for treatment of

attention deficit hyperactivity disorder (ADHD)

INVENTOR(S): Beck, James P.; Pechulis, Anthony D.; Harms, Arthur E.

PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	E A	PPLICATION NO.	DATE
		-		
WO 2002004455	A2 2002	0117 <u>W</u>	O 2001-US21818	20010711
WO 2002004455	A3 2002	0620		
W: AE, AG,	AL, AM, AT,	AU, AZ, BA,	BB, BG, BR, BY,	BZ, CA, CH, CN,
CO, CR,	CU, CZ, DE,	DK, DM, DZ,	EC, EE, ES, FI,	GB, GD, GE, GH,
GM, HR,	HU, ID, IL,	IN, IS, JP,	KE, KG, KP, KR,	KZ, LC, LK, LR,
LS, LT,	LU, LV, MA,	MD, MG, MK,	MN, MW, MX, MZ,	NO, NZ, PL, PT,
RO. RU.	SD. SE. SG.	SI. SK. SL.	TJ. TM. TR. TT.	TZ. UA. UG. UZ.

VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

<u>US 2002091134</u> A1 20020711 <u>US 2001-902845</u> 20010711 PRIORITY APPLN. INFO.: US 2000-217412P P 20000711

OTHER SOURCE(S): MARPAT 136:118393

GΙ

$$R^4$$
 R^5
 R^6
 R^7
 R^7
 R^7
 R^7
 R^7
 R^7
 R^9
 R^9

Title compds. I [R1 = alk(en/yn)yl, cycloalkyl, 5-cycloalkylalkyl and AB benzyl, each of which is optionally substituted with 1 to 3 substituents; R2 = H, alk(en/yn)yl, cycloalkyl, cycloalkylalkyl and haloalkyl; R3 = H, halo, alkyl, haloalkyl and cycloalkyl, wherein alkyl, haloalkyl and cycloalkyl are optionally substituted with 1 to 3 substituents selected from alkoxy and amino; R4-6 = H, halo, alkoxy, NO2, amino, amido, ureido, S(0)n, CN, acyl, carboxy, carboxamide, alk(en/yn)yl, cycloalkyl and cycloalkylalkyl; alternatively R5-6 = O-alkyl-O; R7 = H, halo and alkoxy; X = 0, NH (and substituted derivs.) and S; n = 0 - 2] with some provisos, were prepd. E.g., 7-formylbenzofuran was converted to the corresponding methylamino-Me deriv. (MeOH, MeNH2, NaBH4), alkylated with p-chlorophenacyl bromide (CH2Cl2, Et3N) and reduced to the amino alc. (CH2Cl2, NaBH4, 5 h, $0^{\circ} \rightarrow \text{room temp.}$). This intermediate was treated dropwise with MsOH (CH2Cl2, 0°C → reflux, overnight) to give II as a yellow oil (18% overall yield). synthetic examples were provided. Compds. I are selective neurotransmitter receptor binding ligands (no data). I are useful in the treatment of attention-deficit hyperactivity disorder.

IT 389844-04-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

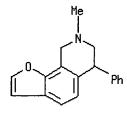
(drug; prepn. and use of furan-fused-4-Ph substituted tetrahydroisoquinolines for treatment of attention deficit hyperactivity disorder (ADHD))

RN <u>389844-04-6</u> HCAPLUS

CN Furo[3,2-h]isoquinoline, 6,7,8,9-tetrahydro-8-methyl-6-phenyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 389844-03-5 CMF C18 H17 N O



CM 2

CRN <u>110-16-7</u> CMF C4 H4 O4

Double bond geometry as shown.

=> file caold

,		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	6.79	155.95
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.65	-0.65

FILE 'CAOLD' ENTERED AT 18:24:41 ON 06 MAR 2003
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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter <u>HELP FIRST</u> for more information.

=> d his

(FILE 'HOME' ENTERED AT 18:22:05 ON 06 MAR 2003)

FILE 'REGISTRY' ENTERED AT 18:22:13 ON 06 MAR 2003

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 6 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 18:24:15 ON 06 MAR 2003

L4

1 S L3

FILE 'CAOLD' ENTERED AT 18:24:41 ON 06 MAR 2003

=> s 13

L5 0 L3

=>

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.80 156.75 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -0.65

FILE 'REGISTRY' ENTERED AT 18:25:51 ON 06 MAR 2003
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STRUCTURE FILE UPDATES: 5 MAR 2003 HIGHEST RN 497055-63-7 DICTIONARY FILE UPDATES: 5 MAR 2003 HIGHEST RN 497055-63-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

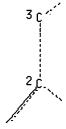
=>

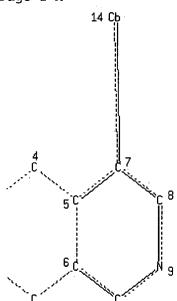
L6 STRUCTURE UPLOADED

=> d 16

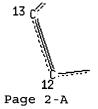
L6 HAS NO ANSWERS

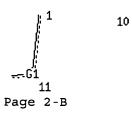
L6 STR





Page 1-B





VAR G1=15/16 NODE ATTRIBUTES: NSPEC IS R \mathbf{AT} NSPEC IS R AT NSPEC IS R AT 2 NSPEC IS R AT 3 NSPEC IS R AT 4 NSPEC IS R AT 5 NSPEC IS R \mathtt{AT} NSPEC IS R AT 7 AT NSPEC IS R NSPEC IS R AT 9 AT 10 NSPEC IS R AT 11 NSPEC IS R AT 12 NSPEC IS R AT 13 NSPEC IS C AT 14

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

=> s 16

SAMPLE SEARCH INITIATED 18:26:10 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2164 TO ITERATE

46.2% PROCESSED 1000 ITERATIONS

1 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

PROJECTED ITERATIONS: 40491 TO 46069

PROJECTED ANSWERS: 1 TO 131

L7 1 SEA SSS SAM L6

=> s 16 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 18:26:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 43040 TO ITERATE

100.0% PROCESSED 43040 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

L8 6 SEA SSS FUL L6

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE

0.00 -0.65

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FILE COVERS 1907 - 6 Mar 2003 VOL 138 ISS 10 FILE LAST UPDATED: 5 Mar 2003 (20030305/ED)

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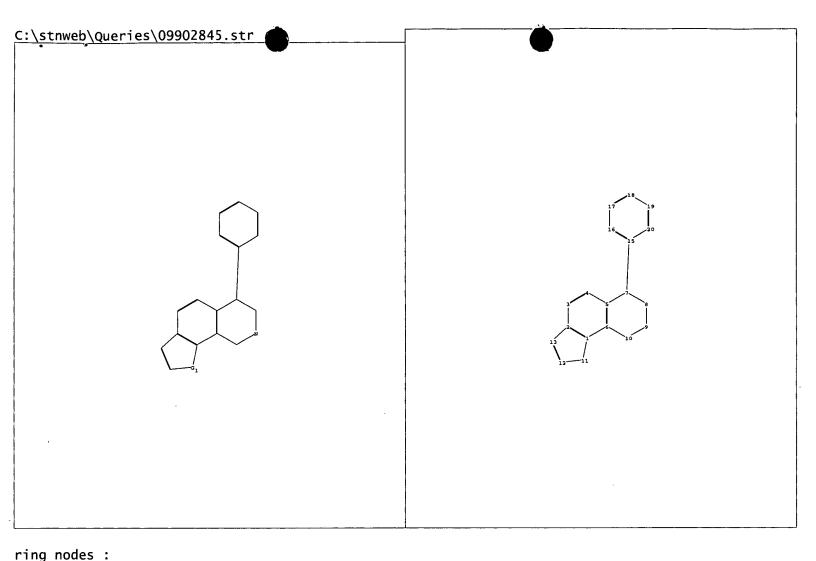
=> s 18

L9 1 L8

=> log y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.25	307.15
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.65

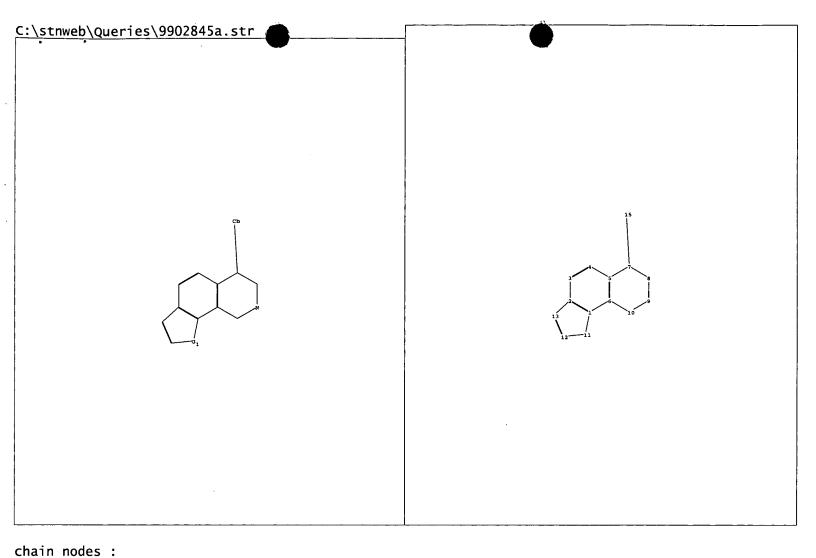
STN INTERNATIONAL LOGOFF AT 18:26:31 ON 06 MAR 2003



```
ring nodes:
    1 2 3 4 5 6 7 8 9 10 11 12 13 15 16 17 18 19 20
chain bonds:
    7-15
ring bonds:
    1-2 1-6 1-11 2-3 2-13 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 12-13 15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds:
    1-11 2-13 5-7 6-10 7-8 7-15 8-9 9-10 11-12 12-13
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20
```

G1:0,S

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom



```
15
ring nodes:
    1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds:
    7-15
ring bonds:
    1-2 1-6 1-11 2-3 2-13 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 12-13
exact/norm bonds:
    1-11 2-13 5-7 6-10 7-8 7-15 8-9 9-10 11-12 12-13
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6
```

•

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 15:Atom